

Rotational spectra of weakly interacting Bose-Einstein condensates

Thomas Papenbrock^a and George F. Bertsch^b

*Institute for Nuclear Theory, Department of Physics, University of Washington, Seattle, WA
98195, USA*

Abstract

We study the spectrum of rotating Bose-Einstein Condensates in the limit of weak repulsive interactions and present analytical and numerical results for energies and wave functions. While the low-lying states are of collective nature, the high-lying states are dominated by single-particle excitations and can accurately be approximated by simple polynomial expressions. In the limit that the number of particles is large compared to the number of excited quanta, the single-particle states become excellent approximations to the eigenstates, and a rather simple ordering scheme is obtained.

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The experimental realization of Bose-Einstein condensation in atomic vapors [1–3] has received much interest in recent years [4]. Very recently experiments have started to investigate Bose-Einstein condensates under rotation. Matthews *et al.* created vortices in a two-component condensate [5], and Madison *et al.* studied rotations of a one-component gas. Theoretical studies have focused on the Thomas-Fermi regime of strong interactions [7–9] or on the limit of weak interactions between the atoms [10–17]. While the former case is closer related to the experiment, the latter case allows for exact (numerical or analytical) solutions and is of particular theoretical interest. Wilkin *et al.* studied the case of attractive interactions [10] and employed a composite boson/fermion picture [12,14] to describe configurations beyond the one-vortex state in few-body boson systems. Mottelson [11] and the Copenhagen group [15,16] analyzed the mean-field theory in the weak interaction limit. In Ref. [13] the authors studied the ground states using exact diagonalization techniques. So far, research has been restricted to the low-lying states in rotating Bose-Einstein condensates. It is the purpose of this paper to study higher excited states in the rotational spectrum.

The Hamiltonian is

$$H = \sum_{j=1}^N \left\{ -\frac{1}{2} \nabla_j^2 + \frac{1}{2} \mathbf{r}_j^2 \right\} + g \sum_{i < j} 2\pi \delta(\mathbf{r}_i - \mathbf{r}_j),$$

where the trap frequency is set to $\hbar\omega = 1$ and g is a dimensionless coupling. In the limit of weak repulsive interactions $0 < g \ll 1$ and maximal alignment of angular momentum with the z -axis the Hamiltonian becomes essentially two-dimensional [11,15]. In what follows we restrict ourselves to this limit and fix the total angular momentum to L .

The problem then consists in diagonalizing the contact interaction in the Hilbert space of degenerate oscillator states at energy total L (setting the ground state energy to zero) [20]. We will analyze the problem in second quantization and in configuration space. While analytical results will be derived in both representations, numerical work is most easily done using second quantization [18,19]. Let us start with the second quantized two-body interaction

$$\hat{V} = \sum_{i < j} 2\pi \delta(\mathbf{r}_i - \mathbf{r}_j) = \frac{1}{2} \sum_{i,j,k,l} \frac{(k+l)!}{2^{k+l} \sqrt{l!j!k!l!}} \delta_{k+l}^{i+j} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l. \quad (1)$$

The operators \hat{a}_m and \hat{a}_m^\dagger annihilate and create one boson in the single-particle oscillator state $|m\rangle$ with energy $m\hbar\omega$ and angular momentum $m\hbar$, respectively and fulfill bosonic commutation rules. For total angular momentum L the Fock space is spanned by states $|\alpha\rangle \equiv |n_0, n_1, \dots, n_k\rangle$ with $\sum_{i=0,k} n_i = N$, $\hat{a}_j^\dagger \hat{a}_j |n_0, n_1, \dots, n_k\rangle = n_j |n_0, n_1, \dots, n_k\rangle$ and $\sum_{j=0,k} j n_j = L$. Here n_j denotes the occupation of the j^{th} single particle state $|j\rangle$.

Turning to configuration space we use complex single-particle coordinates $z = x + iy$ such that $\langle z|j\rangle = \phi_j(z) = (\pi j!)^{-1/2} z^j \exp(-\frac{1}{2}|z|^2)$. Basis functions for the many-body problem are $\psi(z_1, \dots, z_N) \prod_{j=1}^N \exp(-\frac{1}{2}|z_j|^2)$ where $\psi(z_1, \dots, z_N)$ is a homogeneous polynomial of degree L that is totally symmetric in its coordinates. For representations of such polynomials see, e.g. ref. [21]. In what follows we will omit the exponentials when working in configuration space and identify wave functions directly by their polynomial part. Let $\psi(z_1, \dots, z_N)$ be such a polynomial. It is easily seen that the two-body operator

$$\hat{W}_{ij} = \sum_{m,n,k,l} \frac{(k+l)!}{2^{k+l} n! m! k! l!} \delta_{m+n}^k z_i^n z_j^m \left\{ \partial_{z_j}^k \partial_{z_i}^l \Big|_{z_i=z_j=0} \right\} \quad (2)$$

has the same matrix elements as the contact interaction $2\pi\delta(\mathbf{r}_i - \mathbf{r}_j)$. Here it is understood that the derivatives act only onto the polynomial part of the wave function and that they are evaluated at $z_i = z_j = 0$. Performing the sums in eq. (2) and introducing coordinates $R_{ij} = (z_i + z_j)/\sqrt{2}$ and $r_{ij} = (z_i - z_j)/\sqrt{2}$ leads to the following

$$\begin{aligned} 2\pi\delta(\mathbf{r}_i - \mathbf{r}_j) \psi(z_1, \dots, z_i, \dots, z_j, \dots, z_N) &= \hat{W}_{ij} \psi(z_1, \dots, z_i, \dots, z_j, \dots, z_N) \\ &= \psi\left(z_1, \dots, \frac{z_i + z_j}{2}, \dots, \frac{z_j + z_i}{2}, \dots, z_N\right). \end{aligned} \quad (3)$$

Thus, the contact interaction $2\pi\delta(\mathbf{r}_i - \mathbf{r}_j)$ acts on a wave function by replacing the i^{th} and j^{th} argument by its mean value. Note that the center of mass

$$z_c = \frac{1}{N} \sum_{j=1}^N z_j$$

is left invariant under the action of the contact interaction.

Let us now consider the spectrum of states at angular momentum L . States may be classified by their angular momentum quantum numbers L and L_{cm} , and by their energies $E_n = L + g\epsilon_n$. The angular momentum of the center of mass and is denoted as L_{cm} and given by

$$\hat{L}_{\text{cm}} = z_c \sum_{j=1}^N \partial_{z_j} = \frac{1}{N} \sum_k \sqrt{k+1} \hat{a}_{k+1}^\dagger \hat{a}_k \sum_l \sqrt{l+1} \hat{a}_l^\dagger \hat{a}_{l+1}, \quad (4)$$

where the differential operator is understood to act only on the polynomial part of the wave function. The functions z_c and

$$q_k(z_1, \dots, z_N) = \sum_{j=1}^N (z_j - z_c)^k, \quad k \geq 2 \quad (5)$$

are eigenfunctions of \hat{L}_{cm} with eigenvalues one and zero, respectively. Products $z_c^{\lambda_1} q_{\lambda_2} \dots q_{\lambda_N}$ with λ being a partition of L are eigenstates of \hat{L}_{cm} with eigenvalue $L_{\text{cm}} = \lambda_1$ and span the Hilbert space [20] at angular momentum $2 \leq L \leq N$. Note that they do not form an orthogonal basis. Let $|L, L_{\text{cm}}, \epsilon_n\rangle$ denote an eigenstate of the Hamiltonian (1). Due to an $SO(2, 1)$ symmetry one has $z_c |L, L_{\text{cm}}, \epsilon_n\rangle \propto |L+1, L_{\text{cm}}+1, \epsilon_n\rangle$ [22,23]. It is therefore of particular interest to find the “non-spurious” eigenstates (i.e. those with no excitations of the center of mass coordinate) since all other states can simply be obtained by multiplication with powers of z_c [22,10,17]. Figure 1 (left part) shows the spectrum of non-spurious states for $N = 50$ bosons and angular momenta $2 \leq L \leq 18$. Note that there are several high-lying levels that approach constant values as L increases. This is particularly the case for two most energetic levels, and these are well separated from their neighbors for all values of L . As has been observed earlier in exact diagonalizations [13] and mean-field calculations [7,15], the ground states depend linearly on total angular momentum.

Based on numerical results, we suggested in ref. [13] that the ground state wave function is

$$\psi_0(z_1, \dots, z_N) = \sum_{1 \leq p_1 < p_2 < \dots < p_L \leq N} (z_{p_1} - z_c)(z_{p_2} - z_c) \dots (z_{p_L} - z_c), \quad (6)$$

and the ground state energy is

$$\epsilon_0 = \frac{1}{2} \left(N(N-1) - \frac{NL}{2} \right). \quad (7)$$

Very recently, Jackson and Kavoulakis [17] showed the existence of an eigenstate with energy (7) while Smith and Wilkin [24] proved that the wave function (6) indeed has eigenvalue (7). This proof was given using the second quantized form of the interaction. As an application of eq. (3) we now present a shorter proof in configuration space. We expand

$$\psi_0 = \sum_{k=0}^L \binom{N-k}{L-k} (-z_c)^{L-k} \sum_{1 \leq p_1 < \dots < p_k \leq N} z_{p_1} \dots z_{p_k}.$$

Applying operator (2) to this expansion and using the prescription (3) yields

$$\begin{aligned} \hat{W}_{ij} \psi_0 = \sum_{k=0}^L \binom{N-k}{L-k} (-z_c)^{L-k} \left\{ \sum_{1 \leq p_1 < \dots < p_k \leq N}^{\neq i,j} z_{p_1} \dots z_{p_k} \right. \\ \left. + (z_i + z_j) \sum_{1 \leq p_1 < \dots < p_{k-1} \leq N}^{\neq i,j} z_{p_1} \dots z_{p_{k-1}} \right. \\ \left. + \frac{1}{4} (z_i + z_j)^2 \sum_{1 \leq p_1 < \dots < p_{k-2} \leq N}^{\neq i,j} z_{p_1} \dots z_{p_{k-2}} \right\}. \end{aligned}$$

Using $(z_i + z_j)^2 = (z_i - z_j)^2 + 4z_i z_j$ in the third term enclosed in brackets one obtains

$$\hat{W}_{ij} \psi_0 = \psi_0 + \sum_{k=0}^L \binom{N-k}{L-k} (-z_c)^{L-k} \left\{ \frac{1}{4} (z_i - z_j)^2 \sum_{1 \leq p_1 < \dots < p_{k-2} \leq N}^{\neq i,j} z_{p_1} \dots z_{p_{k-2}} \right\}$$

Summing over $\sum_{i < j}$ and using the identity

$$\begin{aligned} \sum_{i < j} \left\{ (z_i - z_j)^2 \sum_{1 \leq p_1 < \dots < p_{k-2} \leq N}^{\neq i,j} z_{p_1} \dots z_{p_{k-2}} \right\} = \\ -kN \sum_{1 \leq p_1 < \dots < p_k \leq N} z_{p_1} \dots z_{p_k} + N(N-k+1) z_c \sum_{1 \leq p_1 < \dots < p_{k-1} \leq N} z_{p_1} \dots z_{p_{k-1}} \end{aligned}$$

one arrives directly at the desired result $\hat{V} \psi_0 = \epsilon_0 \psi_0$.

Another exact result is readily obtained for $L = 4$ and arbitrary N . Employing eq. (3) one may show that

$$\hat{V} \sum_{1 \leq i < j \leq N} (z_i - z_j)^4 = \frac{1}{2} \left(N^2 - \frac{11}{4}N + \frac{3}{2} \right) \sum_{1 \leq i < j \leq N} (z_i - z_j)^4 \quad (8)$$

Unfortunately, we are not able to generalize this result to higher values of angular momentum. Note however that wave functions (6) and (8) comprise the set of non-spurious states for $L = 4$.

Let us consider the most energetic non-spurious state. Numerical computations show that the ansatz (compare with eq. (5))

$$\psi_1(z_1, \dots, z_N) = q_L(z_1, \dots, z_N) \quad (9)$$

has almost unit overlap with the most energetic non-spurious eigenstate and is approaching the asymptotic eigenvalue $\epsilon_1 = \frac{1}{2}(N-1)(N-2)$ exponentially fast with increasing values of angular momentum L . Table I presents numerical values obtained for the overlaps with the exact numerical eigenfunction, energies $\langle \psi_1 | \hat{V} | \psi_1 \rangle$, and widths $\Gamma_1^2 = \langle \psi_1 | \hat{V}^2 | \psi_1 \rangle - \langle \psi_1 | \hat{V} | \psi_1 \rangle^2$. The presented results show that eq. (9) is a highly accurate approximation to the exact eigenstate. This can be understood in more detail by applying the operator (1) to ψ_1

$$\hat{V} \psi_1 = \frac{1}{2}(N-1)(N-2) \psi_1 + 2^{1-L} \sum_{i < j} (z_i + z_j - 2z_c)^L. \quad (10)$$

For sufficiently large L the “remainder” $\sum_{i < j} (z_i + z_j - 2z_c)^L$ is numerically found to have significant overlap only with a small number of eigenstates in the bulk. This explains the quality of our ansatz. Note that $\psi_0 \propto \psi_1$ for $L = 2$ and $L = 3$. Note also that $\hat{V} \psi_1 = [1 + (-1)^L 2^{1-L}] \psi_1$ for $N = 3$. The ansatz (9) describes ψ_1 as an excitation of one particle relative to the center of mass. This picture is confirmed by the computation of selected single-particle occupation numbers $n_j = \langle \psi_1 | \hat{n}_j | \psi_1 \rangle$ shown in Figure 2. The main contribution to the total angular momentum stems from the single-particle orbital $\phi_L(z)$ and a smaller part is carried by the orbital $\phi_{L-1}(z)$. With view to eq. (1) it becomes clear that the energy of ψ_1 depends very weakly on L . The energy contribution of the highly excited single-particle states is exponentially suppressed for sufficiently large angular momenta.

We may also obtain an excellent approximation for the second highest non-spurious state. The ansatz

$$\psi_2(z_1, \dots, z_N) = \frac{N-1}{N} q_2(z_1, \dots, z_N) q_{L-2}(z_1, \dots, z_N) - \psi_1(z_1, \dots, z_N) \quad (11)$$

has almost unit overlap with the numerically obtained exact eigenstate for sufficiently large values of total angular momentum. It approaches the numerically determined energy $\epsilon_2 = \frac{1}{2}[(N-2)^2 - 1]$ exponentially fast with increasing L . Details concerning overlaps and width are presented in Table I. The dominant contributions to the total angular momentum of ψ_2 stem from the orbitals $\phi_2(z)$, $\phi_{L-3}(z)$ and $\phi_{L-2}(z)$. As expected the ansatz (11) describes mainly a few-boson excitation. The single-particle character of the two most energetic states differs strongly from the collective behavior found for the ground state ψ_0 . [11,13,15]. This observation is similar to the case of bosons in the Thomas-Fermi regime [25] and to the case of many-fermion systems like atomic nuclei [26].

We checked that the numerical results agree with ansatz (9) and (11) for various numbers of bosons. The convergence is determined by L only and depends weakly on N . The spectrum depicted in Figure 1 seems to suggest that there are more states which may be approximated by simple polynomial expressions; however we do not see an obvious generalization of the expressions (9) and (11) to account for further states.

Let us consider the regime $N \gg L \sim O(N^0)$ where the ground state is occupied by a macroscopic number of bosons, i.e. $n_0 \sim O(N)$. While low-lying states have been computed in refs. [11,15] we aim at a general understanding of the full spectrum within this regime. Eq. (1) shows that the diagonal matrix elements of \hat{V} are of order $O(N^2)$ while off-diagonal ones are only of order $O(N^{1/2})$. In a first approximation one may then neglect any off-diagonal elements and take the single-particle states as eigenstates. One obtains from eq. (1)

$$\begin{aligned} \hat{V}|n_0, n_1, n_2, \dots, n_k\rangle &= \epsilon_{\{n_j\}}|n_0, n_1, n_2, \dots, n_k\rangle + O(N^{1/2}), \\ \epsilon_{\{n_j\}} &= \frac{1}{2} n_0(n_0 - 1) + 2n_0 \sum_{k>0} 2^{-k} n_k. \end{aligned} \quad (12)$$

Note that typical energies are of the order $O(N^2)$ while energy differences for two different states are of order $O(N)$. Small energy differences may occur for two configurations $\{n_j\}$ and $\{n'_j\}$ that differ only in the occupation of the orbitals $j = 0, 2, 3$. Both configurations should have identical number of bosons and angular momentum, i.e. $n_0 + n_2 + n_3 = n'_0 + n'_2 + n'_3$ and $2n_2 + 3n_3 = 2n'_2 + 3n'_3$. The energy difference of such configurations is only of order $\sim O(N^0)$ which is much smaller than a typical spacing. Thus there are quasi-degenerate levels in the spectrum, and the ground state becomes quasi-degenerate for $L \geq 9$. This observation has also been made by Mottelson [11].

Note that the single particle states have almost good quantum number L_{cm} . One finds $\hat{L}_{\text{cm}}|n_0, n_1, n_2, \dots, n_k\rangle \approx n_1|n_0, n_1, n_2, \dots, n_k\rangle$, and corrections are of order $O(L/N)$. This can be seen by applying the operator (4) to a state with $n_0 \sim O(N)$. Thus, the non-spurious states are comprised by configurations with $n_1 = 0$. We may now discuss the order of the spectrum of non-spurious states. According to eq. (12) this ordering is led by two observations. (i) The lower the number of bosons in the ground state, the lower the total energy of this state. (ii) For two configurations with equal numbers of excited bosons the higher energetic one has the highest single particle orbital occupied. This ordering scheme favors collective motion above single particle excitations. Deviations from this scheme are caused by the quasi-degeneracy of configurations discussed above. The validity of our arguments and of eq. (12) is confirmed by numerically computing and analyzing the spectrum for $N = 46000$ in the regime $2 \leq L \leq 18$.

Let us finally examine the N -dependence of the spectra at fixed L as shown in Figure 3. The spectrum evolves rather smoothly with increasing N and levels tend to be clustered at high N . For instance, there is a triplet of states at lowest energies. This is due to the quasi-degeneracy discussed above, and the triplet is comprised by configurations with $\{n_2 = 6\}$, $\{n_3 = 4\}$ and $\{n_2 = 3, n_3 = 2\}$. Such quasi-degeneracies indicate a high degree of integrability and regularity. However, there are also a few quasi-degeneracies at mid-values of N . Closer inspection reveals that these are avoided crossings. As an example we present in Figure 4 (top) the avoided crossing at $N \approx 70$. The enlargement of the energy clearly indicates an avoided crossing. Further evidence comes from analyzing the wave function structure, i.e. we follow the inverse participation [27]

$$I_\psi = \sum_{\alpha} |\langle \alpha | \psi \rangle|^4 \quad (13)$$

in the basis of single-particle basis states $|\alpha\rangle$. The inverse $1/I_\psi$ measures the number of basis states that have significant overlap with $|\psi\rangle$. Figure 4 (bottom) shows that the wave

function structure changes at the avoided crossing. The simple ordering obtained for the spectrum at large values of N is thus lost when decreasing N . We also recall that avoided crossings indicate some degree of level repulsion and chaoticity [28]. Therefore, we do not expect that all states may be described by simple polynomial expressions. Note however, that the high lying non-spurious states and the ground state do not interact with their neighbored levels – a further confirmation of their regularity.

In summary, we have studied the rotational spectrum of Bose-Einstein condensates in the limit of weak repulsive interactions. The most energetic non-spurious states are well separated from neighboring levels and their energies approach constant values with increasing angular momentum. These states can accurately be approximated by simple polynomial expressions. They exhibit single-particle behavior and differ thereby from the collective behavior of the ground state. In the limit of a macroscopic occupation of the ground state and small total angular momentum the single-particle states become approximate eigenstates. We obtain a simple ordering scheme for the entire excitation spectrum that energetically favors collective behavior over single-particle behavior. This ordering scheme is expected to break down when leaving the limit of $L/N \ll 1$ since some states undergo avoided crossings. While this introduces chaotic behavior in the involved states, the ground state and the highest excited non-spurious states appear to remain simple and regular. Parts of the analytical results presented in this work including a proof concerning the ground state wave function are based on a particularly useful and novel representation of the contact interaction in configuration space.

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- ^a e-mail: papenbro@phys.washington.edu
^b e-mail: bertsch@phys.washington.edu
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TABLES

L	8	12	16	20
$\langle\psi_1 \hat{V} \psi_1\rangle$	1176.325	1176.019	1176.001	1176.000
Γ_1	0.6	0.2	0.03	0.01
$1 - \langle\psi_1 \psi_{\text{exact}}\rangle ^2$	2×10^{-4}	6×10^{-6}	2×10^{-7}	$< 10^{-7}$
$\langle\psi_2 \hat{V} \psi_2\rangle$	1153.031	1151.604	1151.508	1151.501
Γ_2	1.4	0.3	0.09	0.03
$1 - \langle\psi_2 \psi_{\text{exact}}\rangle ^2$	3×10^{-3}	9×10^{-5}	5×10^{-6}	4×10^{-7}

TABLE I. Numerical data for the states ψ_1 and ψ_2 as a function of angular momentum L for $N = 50$. The energy expectation values $\langle\psi_j|\hat{V}|\psi_j\rangle$ approach energies $\epsilon_1 = (N-1)(N-2)/2 = 1176$ and $\epsilon_2 = ((N-2)^2 - 1)/2 = 1151.5$, respectively. The widths $\Gamma_j^2 = \langle\psi_j|\hat{V}^2|\psi_j\rangle - \langle\psi_j|\hat{V}|\psi_j\rangle^2$ are small compared to the level spacing (which is of order $O(N)$), and the overlap with the exact eigenstates is close to one.

FIGURES

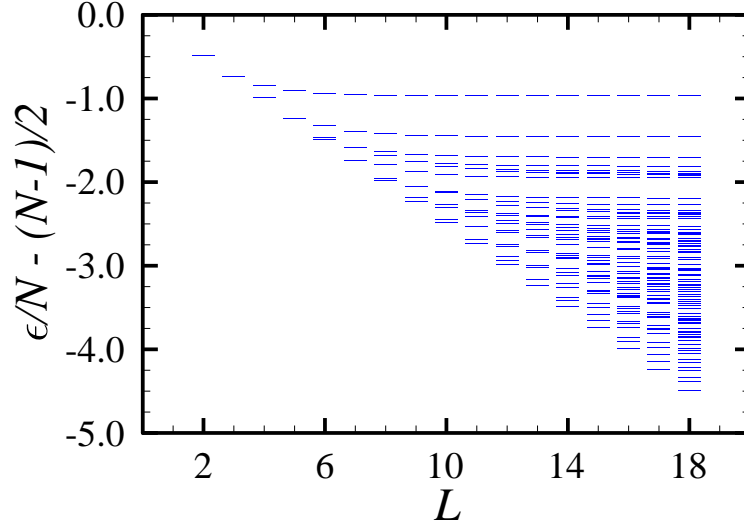


FIG. 1. Spectrum of non-spurious states for a system of $N = 50$ particles as a function of angular momentum.

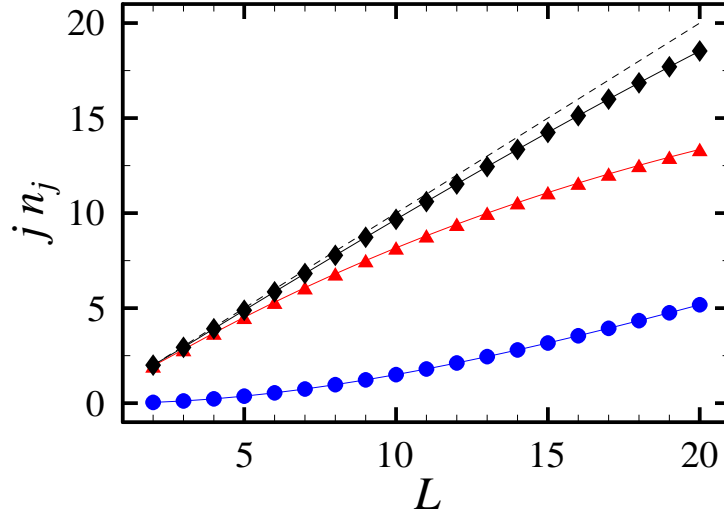


FIG. 2. Structure of state ψ_1 : Single-particle angular momenta $j\langle\psi_1|\hat{n}_j|\psi_1\rangle$ as a function of angular momentum L for a system of $N = 50$ bosons. ($j = L - 1$: circles; $j = L$: triangles; sum of both: diamonds; total angular momentum: dashed line)

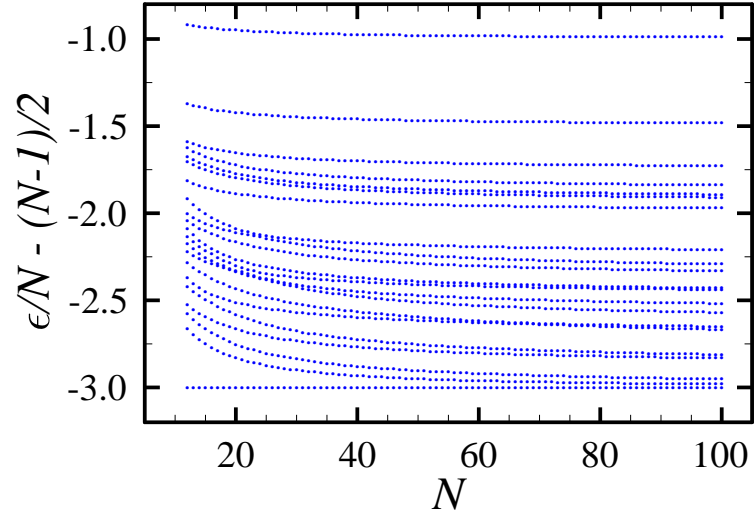


FIG. 3. Spectrum of non-spurious states for $L = 12$ as a function on the number of bosons N .

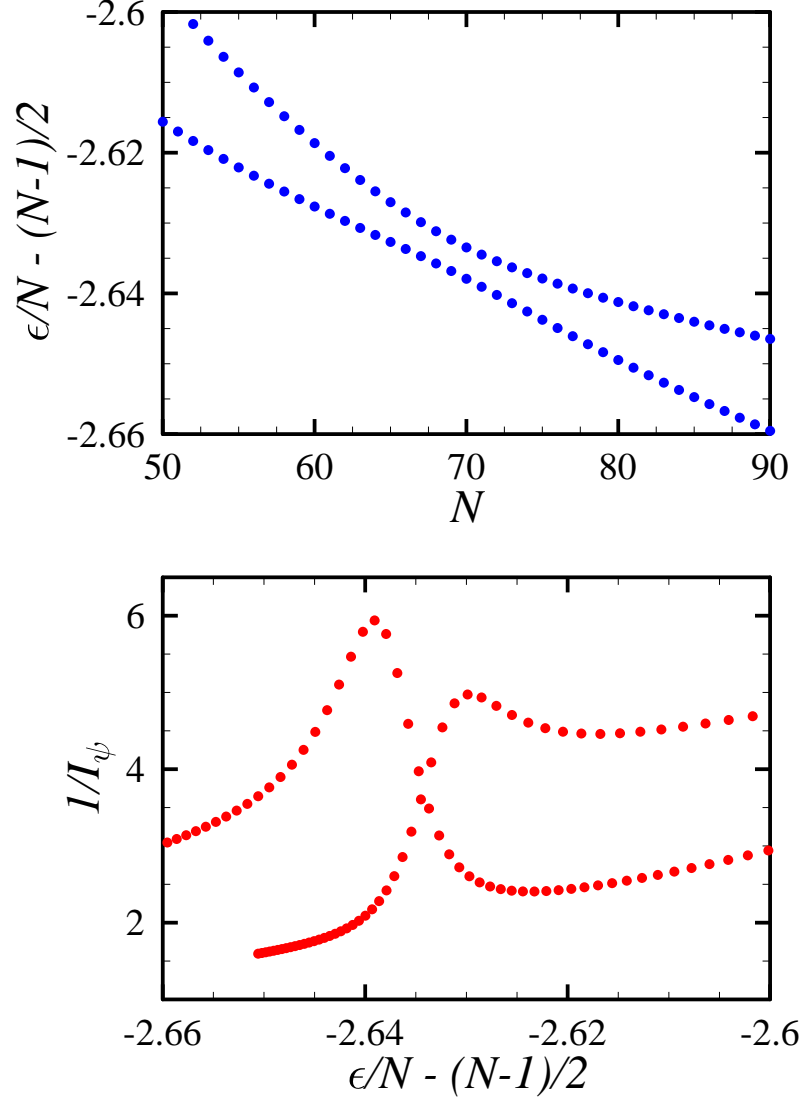


FIG. 4. Avoided Crossing. Top: Two energies as a function of N . Bottom: Number of participating basis states as a function of energy. Results are taken from one avoided crossing at $L = 12$.